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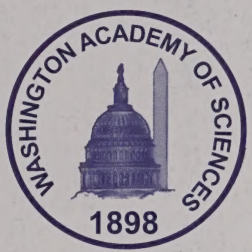

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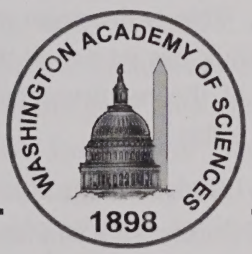

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EDITOR'S COMMENTS

Science today is increasingly driven by data, sometimes massive amounts of raw and processed data. To help with managing this data an initiative in 2016 proposed a set of principles for Findablity, Accessiblity, Interoperablity, and Reusablity (FAIR). In the second article, Gary Berg-Cross and Sage Arbor propose that while the FAIR principles are important, they are still in many ways too simple, and it is necessary to go beyond FAIR to achieve the goals of interoperability and reusability.

The world is complex, consisting of multilevel, nested, interacting systems, their environment, and the boundaries between the systems and the environment. Coping with this complexity requires more than just studying small parts of the world. One must look at the world in terms of wholes and relationships. This is the point of view of the field of systems thinking. Anatoly Levenchuk has surveyed the history of systems thinking and has presented some of the requirements of an ontology for systems thinking as it is practiced today.

In the last article, I look at the problem of computing the locations of "special points" of functions, such as places where the function is zero or has its maximum or minimum value. In my article I develop algorithms for finding some special points that can be useful in some situations and that has some advantages over other algorithms.

This issue ends with the annual Membership List. In addition, there is a section with news articles about members during the past year.

Please send any news about yourselves as well as your comments on papers, suggestions for articles, and ideas for what you would like to see in the Journal to editor@washacadsci.org.

Kenneth Baclawski

Journal of the Washington Academy of Sciences

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4. Include an abstract of 150-200 words.
5. Use Times New Roman, font size 12.
6. Include two to three sentence bios of the authors.
7. Graphics must be easily resizable by the editor to fit the Journal's page size. Reference the graphic in the text.
8. Use endnotes or footnotes. The bibliography may be in a style considered standard for the discipline or professional field represented by the paper.
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Beyond Simple FAIR Principles for Ontologies and Semantic Resources

Grounding Rich, Meaningful Metadata

Gary Berg-Cross[1], Sage Arbor[2]
[1]ESIP Semantic Harmonization, [2]Duke Clinical Research Institute

Abstract

Digital forms of metadata such as controlled vocabularies, taxonomies and conceptual models play an important role in ensuring that data satisfy the principles of findability, accessibility, interoperability, and reusability (FAIR). In turn, metadata also relies on semantic artifacts called formal ontologies to make metadata computer processable. Ontologies make metadata semantically rich with axiomatized definitions that represent useful meanings, but adapting simple ideas of FAIRness for a broad class of digital objects called semantic resources, especially ontologies, raises a number of semantic issues. The focus here is on issues involving community standards for rich metadata and adequate grounding of these with meaningful semantics. This comes despite the fact that in many ways, ontology developments have preceded, and proceeded well beyond, simple FAIR principles. We illustrate the value of community standards by the development of capabilities to document ontology modules sharing a common framework. As part of grounding semantics, we suggest a useful direction is to capture the form of axiom patterns using common ontology design patterns, which are themselves grounded in foundational concepts.

1. Introduction

SCIENCE, ESPECIALLY OPEN SCIENCE IN A DIGITAL AGE, is increasingly data driven, relying on integrated data access via the Web. This open science strategy to use information artifacts has long been challenged by the heterogeneity of big digital data and has led to increased reliance on metadata to support finding, understanding and using relevant managed digital data. As an aid to data management, the FAIR initiative (Wilkinson et al., 2016), with four foundational principles for Findablity, Accessiblity, Interoperablity, and Reusablity, has gained significant traction. FAIR principles provide, for example, some guidance on metadata practices to support open data access and operation (Blomberg et al., 2016). An important feature of the FAIR principles is to go beyond simple metadata using key-value pairs that describe basic characteristics found in typical,

published datasets. Examples of simple metadata are tags for titles, identifiers, text descriptions, keywords, publisher name, date of publication, or terms of use. Databases such as the Disease Database (2022) are illustrative of using this simple type of metadata to document data.

The FAIR foundation and more detailed guiding principles grew in part out of the recognition that the vocabularies needed for metadata should be standardized and further that some semantics is needed to enable machine-actionability (i.e., the capacity of computational systems rather than humans to find, access, interoperate, and reuse data). Partly in response to the useful role of FAIR principles many diverse semantic resources and knowledge graphs (KGs) have been developed across the domains. These domains are as varied as the biomedical and earth sciences. KGs are very popular as useful integration artifacts because they in effect turn related pieces of data into actionable knowledge units (De Smedt et al., 2020).

To help with such things as data integration used in KGs, FAIR includes rich metadata as a central concept as well as some metrics to help objectively score FAIRness. This highlights the dependency of FAIR data on appropriately rich, community agreed upon metadata. Such metadata starts with FAIR vocabularies that are linked and have formal semantics to allow automated processing (Figure 1). Another central feature, illustrated in Figure 1, is that FAIRness is recursive with the role of FAIR metadata at its level requiring some more fundamental grounding in a richer level.

So FAIR vocabularies need to be grounded in FAIR ontologies. These are the ones obeying FAIR principles like findability. But how is FAIRness assessed?

As an aid FAIR provides some best practices of metrics for data/informational resources (Crosswell, 2022). Metric tools, like self-assessment instruments and validators, were developed early on (Wilkinson et al., 2018; Devaraju et al., 2021) to generate a global FAIRness score. But as work on FAIR has progressed it was recognized that the original technology neutral concept of self surveyed "metrics," involved a degree of subjective interpretation. This threatens the idea of adequate grounding of metadata for both machine processing and human understanding. The response has been to develop several more objective measures called "Maturity Indicators" (FAIR Maturity Indicator, 2019). Essentially maturity indicators

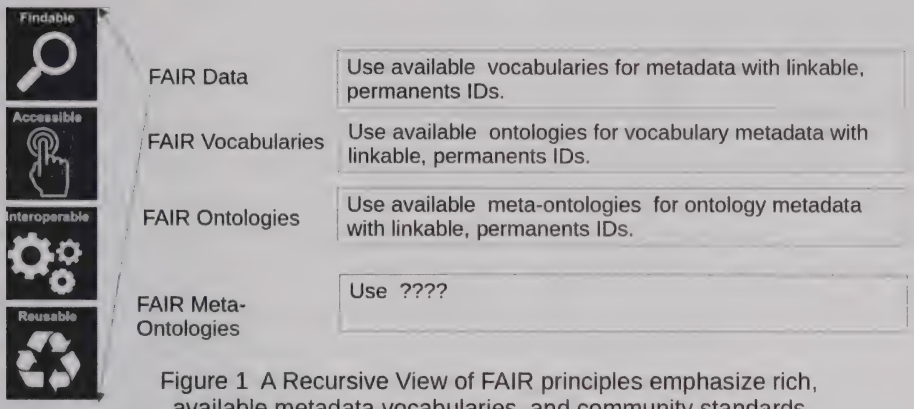

Figure 1 A Recursive View of FAIR principles emphasize rich, available metadata vocabularies and community standards

describe the various components of FAIRness in operational ways that can be objectively evaluated by semantic technologies tools (RDA, 2020). For example, the first maturity indicator for findability, checks that a repository implements accessible, structured metadata to enhance its discoverability on the Web. This is essentially an existential check that a globally unique and permanent identifier (GUID) has been used to name a data element and that an associated link can be resolved. The presence of any Linked Data that can be found for a data element is then considered an objective success (FAIR Maturity Indicator, 2019). A similar idea is adopted for metadata. The metadata maturity indicator is an existential check that metadata follows some "community-defined model."

In both cases there is a degree of simple objectivity, but, on reflection, one might ask whether we have measured everything of interest and in particular the meaning understood for vocabulary terms serving a metadata role. There is, for example, no unique definition for "soil" or "soil density," and so there may be many different, but unique, GUIDs for a named term in a vocabulary, defined in a vocabulary glossary and/or data using the vocabulary label "soil." Similarly, a community standard may exist for defining particular metadata items, but the quality of this standard, especially older standards that are not actively maintained, may vary in important ways.

As an example, Maron and Feinberg (2018) discuss the importance of the way that standards creators, like the Dublin Core standard, understand what it means to "adopt a standard." This is different from the way that web publishing platform implementations share digital collections as well as how regular users understand what it means to "adopt a standard."[1] A key point here is that there can still be an uncomfortable degree of subjective understanding of maturity indicators and what a particular guideline means. This highlights the centrality of semantic meaning in grounding FAIRness. Unfortunately at the domain level (e.g., what is soil density?), the required data vocabularies to use for some domain's metadata are currently little more than lists, while others contain arbitrary definitions. This lack of domain definitions that have good quality and are accepted by the community is clearly a problem for FAIRness. Further, vocabularies limited to human readable text do not follow the encouraged FAIR practice for metadata schemes, implied in Figure 1, which is to use a formal, accessible, shared, and broadly applicable language for knowledge representation based on semantic models such as formal ontologies (Guizzardi, 2020). If, for example, vocabulary can be described with measurable units (e.g., soil density as kg/m^3), more robust universal definitions are possible. However many vocabulary words do not encompass such units in their meaning.

Ontologies, with standardized lexicons that include information about how items are categorized and related to one another, play a role both in building KGs and in supporting FAIR data principles. Such ontologies can provide semantically defined vocabularies usable for what FAIR calls rich metadata annotations for data. The relations in Figure 2 illustrate how vocabulary standards, such as SoTerML (Pourabdollah et al., 2012) and ontologies, such as GloSIS (Palma et al., 2020), further enrich the data-metadata associations by embedding a particular concept within a related conceptual pattern or schema.

It has long been understood that some degree of useful semantic interoperability can be achieved by leveraging formal ontologies that capture meaningful conceptualizations and that can be shared as digital artifacts. As part of the Semantic Web initiative, Heflin and James Hendler (2000), for example, described the challenge of meaning-based data integration:

[1] A sign of how difficult it is to maintain links is the fact that FAIRsharing's list (https://fairsharing.org/standards/identifierschema) of community-recognized identifier schemas has a broken link.

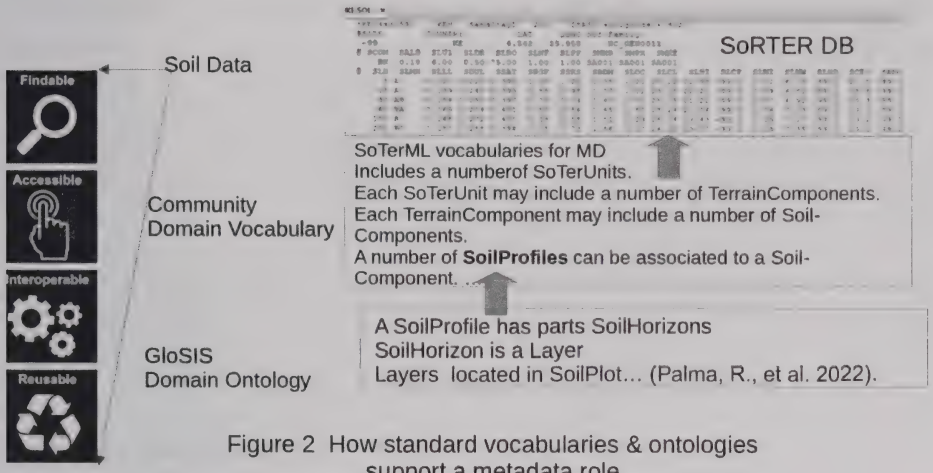

Figure 2 How standard vocabularies & ontologies support a metadata role

> To achieve semantic interoperability, systems must be able to exchange data in such a way that the precise meaning of the data is readily accessible and the data itself can be translated by any system into a form that it understands.

However, the Semantic Web's vision of easy interoperability has not been widely achieved in the intervening years. While simple conceptual definitions such as seen in Figure 2 can serve as links between different data, there is no one, master, ontologically formalized conceptualization. Rather there are as many ontologies as there are vocabularies defining conceptualizations of data in different ways. This reflects that fact that humans understand and define a concept, such as with the label "soil," in many different ways. Thus ontologies that are structured using vocabulary definitions also come to reflect different understandings. While the word "soil," for example, is conversationally used and understood in what seems a common, conceptual space there is no universally recognized, precise definition. Contexts like agriculture evoke different conceptualizations of soil because they emphasize things like manure as a constituent beyond the more typical constituents of sand and clay. Vocabularies, like ontologies, may have implicit scope, but still may be understood by different people based on their role relations to the domain being formalized. Even more conceptual differences can be found, including the implicit meanings evoked by

the topic of "soil liquefaction" or "soil contamination" (Todd-Brown and Berg-Cross, 2022).

Recognizing that meaning can change subtly in the relations found in different contexts encourages the use of supplementary semantic methods which go beyond creation of a simple conceptual model. These include standardizing and aligning definitions to help clarify extant conceptualizations, which can in turn support finding and using appropriate labels backed by community standard definitions for data. Thus connecting a basic concept of "soil" with usual constituents to a sub-concept of "toxic soil" with hazardous ingredients allows greater coverage across the wide conceptual space that people understand about soils.

So a simple application of ontologies does not solve all the problems of data and meaning with respect to a domain. Thus researchers have considered the FAIRness issues for ontologies themselves. This makes sense since, as seen in Figures 1 and 2, FAIRness applies to metadata and some of that FAIRness relies on ontologies. However, some problems for ontology FAIRness are illustrated by a recent survey on disaster management ontologies by Mazimwe et al (2021). They performed FAIRness tests using published information available as part of a review and found that FAIR principles were seldom followed for many of the ontologies analyzed. Surprisingly the average Findability[2] using the four FAIR Finding criteria was only 1.8%, and the average Accessibility, which is provided by functioning APIs, was only 5.8%. Only 4.3% of the retrieved ontologies provided details about explicit mapping/correspondences between ontologies. Metadata schema issues were also reported by Mazimwe et al (2021) such as a failure to use standard vocabularies to describe semantic artifacts. And rather surprisingly 90.9% of URLs provided for the artifacts did not conform to the well understood principle of uniqueness and persistence of links.[3] Some of the lack of resolvable URLs may reflect "link rot" and the fact that older (pre-2015 and hence pre-FAIR principles) ontologies were included. Thus for a number of reasons it seems useful to examine some issues about FAIR ontologies, especially semantic and community issues that may involve more than simple ideas of FAIRness.

[2]Findability involves assigning unique and persistent identifiers to a digital object, and describing them with rich metadata that enable their indexing and discovery.

[3]The first access principle requires that (meta)data are retrievable by their identifier using a standardized communications protocol.

This paper discusses examples of community standardization efforts, technologies and methodologies for developing FAIR ontologies and takes a deeper look at ontology metadata and how harmonization across the semantic spectrum is needed to facilitate semantic interoperability. The remainder of the paper is structured as follows. Section 2 provides context and illustrates some work and issues arising from a simple application of FAIR principles to ontologies and the automation of meaningful metrics. In Section 3 we provide some examples of independently developed guidelines for metadata documentation of ontology characteristics and content. Section 4 presents a biomedical example of FAIR ontologies in the complex COVID-19 domain and illustrates the value of a coordinated, community effort to build related and interoperable ontologies. Section 5 concludes the paper by examining the problem of grounding metadata so that it has the rich semantics that is necessary for achieving the FAIR principles and beyond.

2. Applying FAIR Guiding Principles to Ontologies

As context, some examples of FAIR ontology work is provided to help understand some of the issues involved in finding, accessing and sharing ontologies. We start with the idea of rich metadata used for ontologies. We leverage rich metadata guidelines and methods that were developed for the FAIR principles before looking at semantics beyond FAIR.

Ontological challenges relating to FAIRness, for whatever purpose, start with finding one or more relevant ontologies and drilling down to concept(s) within the ontology[4]. Providing rich metadata describing ontologies in a meaningful way is essential for finding an ontology[5]. We can see how this works from a FAIR perspective by simply replacing the concept of "data" with "ontology" in FAIR guidelines (Poveda-Villalón, María et al., 2020). This give us an aspirational start on finding relevant ontologies and their conceptual elements using guiding principles:

FO1 Ontologies (and their elements) are assigned a globally unique and persistent identifier.

[4]Finding and accessing knowledge are closely related in deciding which ontologies to use and are discussed together in this subsection.

[5]There is an obvious degree of recursion here since metadata describing an ontology must itself be FAIR and such vocabularies should be grounded in fundamental concepts about ontologies.

FO2 Ontologies (and their elements) are described with "rich" metadata (meta-ontologies[6]).

FO3 Ontologies (and their element's) metadata clearly and explicitly include the identifier for the ontology/elements they describe.

FO4 Ontologies (and their elements) are registered or indexed in a searchable resource.

FO1 reflects principles like universal identifiers and resolvable linkages. Ontologies have long included some such practices to help find and access their contents. Guidance to find elements was part of the earlier Linked Data principles growing out of the Semantic Web in 2006. Before the widespread acceptance of FAIR principles for data research there were Linked Data guidelines along with experience publishing ontologies on the Web using permanent identifiers and making them available through the HTTP protocol (Janowicz et al., 2014). Despite this, as Mazimwe et al (2021) have shown, even easy practices such as resolvable GUIDs may not always be followed.

FO2 requires metadata about an ontology, most importantly what its content is. Part of the early work with ontology repositories demonstrated the lack of community agreed upon metadata standards for fully describing even the basic content of ontologies. Dutta, Nandini and Shahi (2015) observed, for example, that while the majority of ontology libraries/repositories used the term "author" to capture authoring information of an ontology, some of the early libraries used the term "creator." This seems simple to fix with linguistic concepts like "synonyms." But other meta-aspects of rich metadata, such as how to describe an ontology's content and structure to find a relevant ontology, are more difficult to agree on and implement.

Richness can be subjective and thus some of what humans find satisfyingly rich based on available background knowledge can be hard to formalize for computer processing. Some knowledge represented in, say an ontology schema, might provide a useful index to find a relevant ontology. But there is yet no universally agreed upon schema to represent the complexity of a particular ontology's content. Instead, any checking to find

[6]There is an obvious recursion in richly describing ontologies by other ontologies having a meta-ontology role.

an appropriate ontology (or another semantic resource like a controlled vocabulary) typically requires considering characteristics, such as quality of defined meanings. These are characteristics that make an ontology relevant, trustworthy and useful.

Simple ontology search tools do exist to use for some domains such as biomedical topics (The Ontology Lookup Service, 2022). But they are built to find a relevant concept based on a label like "disease" or "soil." And while a list of candidates may be provided by such a simple search, further analysis of candidate ontologies is usually needed. For example studying taxonomic structure is important, which in turn requires access and analysis (Jacobsen et al., 2020).

Use of metadata for interoperability is even more challenging than finding separate but related ontologies. To start, we require APIs between the repositories containing the ontologies. Moreover, these APIs may need to access other ontological knowledge, possibly in other repositories, because ontologies, like data and metadata, are distributed. How does metadata tell us about what axiomatized information can be shared? How does an automated operation tell that two definitions are equivalent or even compatible?

We can provide a start on simple guidance for this type of operation by simply translating three FAIR data interoperability principles to ontologies and see where they lead. We then have:

IO1 Ontology metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation across different ontologies. As part of a Semantic Web vision, the original interoperability guidance was simple. The idea was to use metadata vocabularies that conform to the major available logic-based knowledge representation languages (Berners-Lee et al., 2001). Unfortunately this ignores the content of what is represented.

IO2 Ontology metadata use controlled vocabularies that follow FAIR principles.

IO3 Ontology metadata includes qualified references to other ontology metadata.

More experience with data interoperability has led to growing requirements beyond the guidance of IO1 to just semantic language standards

or even a direct use of ontologies represented in these languages. However, the principle of "garbage in-garbage out" still applies, even if the representation language of an ontology allows automated processing. The quality of what is represented in an ontology is what is important here and not just the representational language.

Because there is no one master ontology to represent everything, there is a need to interoperate between ontologies, guided by what we know of them from IO2 and IO3. While there may be existential items that can be checked from a meaning point of view, this is shallow and not rich metadata. One can argue that we need more meta semantics as we move to consider how to support interoperability of related ontologies, which are increasingly stored, like data, in repositories. Deeper, rich documentation here involves relating concepts. These may be captured in ontology mappings, alignment and even harmonization. But this can be hard and a common approach is to simplify interoperability often to something like a word-based shallow alignment between ontologies. One example of simple alignment uses the Simple Knowledge Organization System (SKOS), which is based on labels and/or a simple thesaurus scheme. SKOS represents similarity of terms using linguistic or hierarchical representations like "broader term" or loosely associative ones like "related terms" as opposed to richer representations of semantic relations like "same class as." While the SKOS vocabulary is shallow, it is useful because it is formalized in a Resource Description Framework (RDF) processable format. This provides at least an entry step to an incremental semantic approach, which allows for subsequent work to expand the scope and to provide richer domain semantics (Berg-Cross, 2021).

3. Beyond FAIR to Richer Metadata Vocabularies for Ontologies

Ontological methods have something to contribute beyond the FAIR guidelines. Interestingly, standardizing metadata for ontologies has followed an incremental path to maturity that is a bit independent of, and partly precedes, the FAIR initiative. To some extent this independent path may have made ontology developers less motivated to use simple FAIR ideas for ontology development and documentation. Here we can agree with Amdouni, Bouazzouni, and Jonquet (2022) that we have yet to see a clear methodology implemented and tooled to automatically assess the level of FAIRness to ontologies. But in some ways, even without common,

tooled methods, we have worthwhile resources to take a few steps toward rich metadata for ontologies.

An initial step towards a standardized metadata vocabulary was taken with development of the Ontology Metadata Vocabulary (OMV) by Hartmann et al. (2005). The work provided a broad, if not deep, view of key metadata requirements, which, in part, both prefigure FAIR principles by some 10 years (the ones overlapping with FAIR are emboldened below) and include semantic aspects beyond initial FAIR principles.

Eight factors were developed as listed below, and a few highlights are worth noting. One is that OMV includes factors like usability for humans. But as a formal semantic effort it also provide guidance on making the models processable. Another is that it includes an important distinction between the rationalized conceptualization underlying ontological development and the pragmatics of how an ontological model might be realized in ways that are helpful for a range of users. Another important idea is that it lists some minimal documentation of key information.

1. **Accessibility**. Ontology metadata must be accessible and processable for machines as well as humans.

2. Usability. The metadata should be understandable so that a majority of domain users should be able to readily apply metadata.

3. **Reuse**. Because ontologies are a (or the) core technology for the Semantic Web, its metadata should reflect key issues of the Semantic Web such as reuse and sharing of knowledge.

4. Conceptualization vs. Realization. Metadata must reflect a distinction between the underlying semantic conceptualization and its particular realization as a concrete ontology digital artifact.

5. **Interoperability**. Metadata interoperability is key and was defined as conforming to the major representation languages being used for Semantic Web applications in 2005, such as the Web Ontology Language (OWL).

6. Documentation. Metadata documentation should provide at minimum information about technical, statistical, accessibility, management information, etc.

7. Extensibility. Reflecting special user needs and the reality that on-

tologies are built incrementally as knowledge requirements and issues unfold, it is required that beyond such standard metadata, facts can be added and extended easily.

8. Expressiveness. Metadata must be expressive enough to represent all desired aspects, as presented above.

With the growing impact of ontology repositories between 2005 and 2014 the wide, principled scope of metadata, the proposed OMV needed more detail to guide behavior. OMV was followed by a more detailed de facto guideline called "Metadata for Ontology Description and publication" (MOD) (Dutta, Nandini and Shahi, 2015). This reflected the actual experiences to find and share relevant ontologies in repositories such as BioPortal. MOD's guidance concerns how to document ontology characteristics and contents so that they are easily identifiable and reusable for various knowledge engineering tasks. These documentation requirements were derived from a bottom-up survey of repository searches, which identified detailed and specific properties used in ontology repositories. As a result of their survey and analysis, Dutta, Nandini, and Shahi (2015) also proposed eight requirements for ontology documentation. These partially overlapped with OMV's metadata requirements (such as Extensibility and Usability):

1. Brevity: The vocabulary should consist of a minimal set of elements maintaining balance between necessity and sufficiency.

2. Clarity: The metadata elements must be well defined, and clear descriptions should be provided.

3. Simplicity: The vocabulary should be easy to use.

4. Authority: The vocabulary design should be based on a sound methodology in the sense that the inclusion of terms in the vocabulary are justified.

5. Standardization: The element names should be standardized. To confirm the standardization, the individual elements should be mapped with the existing standard vocabularies.

6. Extensibility: The vocabulary should be extensible.

7. Usability: The vocabulary should support the reuse of the described resources. In other words, the vocabulary should allow the creators/developers to highlight the usage and the quality of the resources

in a well-defined manner.

8. Interoperability: The vocabulary should be interoperable. That is, it should conform to the major knowledge representation languages then in use for Semantic Web (Berners-Lee et al., 2001) applications.

As with FAIR principles there are issues with objectivity of the guidance. Characteristics like "brevity" and "clarity" are comprehensible to humans, but there is no easy guidance to make the brevity of metadata quantifiable. From a process point of view, what are well defined and clear descriptions? Further, principles like standardization of vocabularies do not address the quality of a vocabulary. More immediately helpful to documenting ontologies with metadata was MOD's use of seven metadata facets that include aspects like a basis for *Authority*, along with *Rights* and *Licenses* needed for ontological use. MOD facets are populated using 15 classes[7] that are formalized and expressed in the Web Ontology Language and thus processable[8]. The classes were derived by analyzing top-level facets such as *Authority*. For instance, the *Authority* facet identifies the person/organization that created the ontology and/or who exercises control over an ontology, or originated an ontology document. MOD semantics considers both *Person* and *Organization* as classes and these are grouped under a general class called *Agent*. The *Environment* facet includes classes like OntologyTool, OntologyLanguage, and OntologySyntax (Dutta, Nandini, and Shahi, 2015).

Perhaps the most interesting top-level facet is *domain coverage*. This often describes technical metrics about the ontology, such as the number of classes and properties, and the scope, which include requirements and a standard practice for developing ontologies called community competency questions (Aminu et al., 2020). Documenting competency questions takes metadata well beyond simple FAIR guidance. While a pattern of classes might be used to define a domain, often this is shallowly abbreviated with a label such as "protein" or "soil." But if reference is made to an ontology, a processable definition with axioms can be available and instances of a domain can be defined using RDF schemas. This is much more in the style of rich metadata, and we can see below an example of

[7]A class is a conceptual collection of things that share common attributes.

[8]Note that this was done several years before the FAIR standard and reflects earlier emphasis from the Semantic Web.

an axiomatized definition in the Environmental Ontology (ENVO) using standard relations also found in various other ontologies.

For example, Soil
is a type of environmental material
has quality some porous
has part some sand
has part some organic material
has part some mineral material
has part some (chemical entity and (has role some nutrient))
part of some pedosphere
has part some clay
has part some silt

MOD has been used successfully as part of ontology development, but the range of possible metadata growing out of MOD's suggestions is large. Agro-Portal, for example, now recognizes 346 properties from existing metadata vocabularies that could be used to describe different aspects of ontologies and other semantic resources (Toulet, Dutta, and Jonque, 2018). This is rich in number but not always in depth. So choosing which metadata vocabulary items to use can be an issue.

A further tuning of documentation requirements provides some idea of which elements are essential as part of publication and/or in ontology repositories. The Minimum Information for Reporting an Ontology (MIRO) initiative, associated with the Open Biomedical Ontology (OBO) Foundry, provides guidance for what ontology developers should document about an ontology (Matentzoglu et al., 2018). If MOD was aimed at improving ontology repositories, MIRO added a goal of what should be documented in scientific reports. The MIRO guidelines specify the level of importance using a "must," "should" or "optional" label for each element as an aid to improving the quality and content consistency of the information descriptions. This further constrains the variability in descriptions of ontologies. At a minimum, for example, developers must describe the development methodology, provenance and context of information being reused. MIRO defines 34 information items, some of which, such as "ontology name", "ontology license" and "ontology URL," are content-independent, i.e., do not depend on what an ontology is about. They are thus not really rich metadata, although they will have GUIDs that are resolvable.

The MIRO work is significant, but as noted by Amdouni, Bouazzouni, and Clement Jonquet (2022), MIRO properties are not explicitly aligned with FAIR principles and assessment methods. In reality MIRO's 11 guideline items for ontology content go beyond FAIR and have been of importance for supporting ontology standardization and interoperability. In particular two guidelines go deeper than FAIR and were considered very important for users. These are information about ontology relationships and about axiom patterns. Both can be seen in the example of an axiomatized definition for soil. Guidance for relations and patterns reads as follows:

> **E.9** Ontology relationships and properties used in the ontology must be documented.
>
> **E.10** Axiom patterns must be documented. An axiom pattern is a regular design of axioms or a template for axioms used to represent a category of entities or common aspects of a variety of types of entities. The previous example of an axiom pattern used to define "soil" illustrates this.

In ontology tools like Protégé one can see and select from defined relations needed to implement E.9. Examples are *part*, *participation* and *composition* relations. In the OBO Foundry, for example, one may see a list of available relations stored in the Relations Ontology module (OBO Relation Ontology, n.d.). A *participation* relation, for example, has sub-types such as *input_of* to further specify the nature of participation. Metadata documentation of relations and axioms makes it possible to understand how concepts are conceptualized and represented. Documenting axiom patterns with a canonical set of Ontology Design Patterns takes one even deeper towards ontology interoperability, since the use of a common design based on good practices provides a common point for both development and inter-operation.

To help start ontology development one can search various catalogs of ontology design axiom patterns. These can be used as starting points for ontology development (ODP, 2022). Ontology design patterns are largely hand crafted because computationally extracting axiom patterns from an extant ontology remains difficult. However, early attempts have been made, such as extracting syntactic regularities from ontologies as proxies for axiom patterns (Mikroyannidie et al., 2011).

More recently, the Shapes Constraint Language (SHACL) standard and SHACL shape graphs provide a description of data graphs satisfying particular configuration conditions. This means one can define model shapes using vocabularies that are themselves defined and expressed in RDF graphs. In turn SHACL-defined shapes can be tied to the shape of ontological concepts and ontology design patterns because particular ontology design pattern axioms describing conceptual constraints on instances operate in a similar fashion to SHACL-generated constraints. Thus, closing the loop, an argument has been made that the structure of ontology design patterns might be used as an empirical basis for SHACL shape graphs (Pandit et al., 2018). This might afford some automated documentation of axiom patterns (Cimmino et al., 2020; Blomqvist et al., 2021) and provide a deeper basis for objective and processable axiom patterns used to describe ontology concepts.

An important distinction among ontologies is whether the ontology is intended to deal primarily with concepts or with data. The former kinds of ontologies will contain logical statements framed in terms of domain attributes and how they define the meanings of things in that domain (Bennett, 2021). These logical statements can be used by humans to understand things in the domain and to explain more complex collections of inter-related things. When things in a domain need to be represented with data, the ontology is often known as an "operational" or "application" ontology. Since the FAIR principles are concerned with data, it would seem that the only ontologies that would matter for FAIR are ones that deal with data. However, further analysis suggests that there may be different styles of ontology that deal with operational data. An ontology for integrating multiple sources of data may need to have more semantically nuanced distinctions to deal with the different ways those data sources reflect conceptualizations of the world. On the other hand, an ontology for reasoning over data (e.g., in a knowledge graph) would typically be simpler (Baclawski et al., 2021). Furthermore, even an ontology that is purely conceptual must still be represented using data (e.g., in OWL or first-order logic), and so the FAIR principles are relevant to the ontology itself.

There are other differences between operational and concept ontologies. For example, an operational ontology need not use a full foundational ontology to partition its world. It would also typically have fewer relationships, with little or no use of constraints such as property domains and

ranges. By contrast, a concept ontology would have a richer set of relationships such as for different types of whole-part relations, and would reflect the many constraints that apply to the relationships and properties.

Any metadata that is intended to be used for findability and reusability needs to recognize and accommodate the distinction between conceptual and operational ontologies as well as distinctions among different styles of operational ontology. Otherwise an ontology developed to define real-world meanings may get re-used in an ontology application for data processing, with generally bad results. The intended use of an ontology is an example of an ontological commitment. In a similar vein, metadata should be included for other ontological commitments, such as realism and 4D "extensional" ontologies[9].

4. Scoping the Community Role in Quality Ontologies

As we have seen there is a need for richly developed vocabularies to describe a given domain. Perhaps no domain has systematically developed findable ontologies to support data use more than the biomedical field (Smith et al., 2008). A good biomedical community example is what has been developed as part of the OBO Foundry (OBO, n.d.). Besides a large user base and consistent management activity, the OBO Foundry Tools feature operational rules that are easy to find and access, along with a suite of automated tools to validate rule compliance and a dashboard for easy understanding on an ontology's degree of conformity with each principle (OBO Foundry Tools, n.d.; Jackson et al., 2021). Taken as a whole this work illustrates:

- principles and practices to ensure that relevant biomedical ontologies are findable.
- the use of a modular approach to support alignments and extensibility, and
- systematic axiomatizations of concise definitions that users may use for search.

When properly executed by a sizable, federated community, these principles can help improve overall quality and interoperability between ontologies

[9] A 4D ontology regards individual objects as being four-dimensional, having spatial and temporal parts, and existing immutably in space-time.

whose use in turn supports the goals of FAIRness.

Starting with the first principle above, one may find relevant conceptualized biomedical and associated domain vocabularies to make data FAIRer just by using the OBO registry (OBO Registry, n.d.). Here one finds persistently available, versioned copies of ontologies represented in OWL that are accessible using standardized interfaces. Protocols for retrieving well managed ontologies from repositories like BioPortal and the OBO Foundry are explicit and easy for both humans and machines. Furthermore, storage of ontologies on GitHub repositories include well-defined mechanisms to obtain authorization for access to versioned ontologies.

Of great importance is finding information about an ontology's coverage and scope. This essentially concerns the relevance of an ontology and what it claims to cover (Matentzoglu et al., 2018). In practice, as noted earlier, finding a relevant and accessible ontology requires good searching skills and experience followed by consideration of what is known about the ontology. General guidance for creating rich metadata, in the form of meta-ontologies, and registering them in trustworthy repositories can also help with other FAIR principles such as accessibility. But, as we have seen, there are a wide range of approaches to metadata for ontologies. Accordingly we should add richer information such as taxonomic classes and property relations, which may facilitate data integration and interoperability, and whether a state-of-the art, general ontological methodology or framework has been used[10].

A good illustration of such considerations in the biomedical domain was driven by the COVID-19 pandemic. This pandemic challenged healthcare systems and research worldwide as worldwide data was collected, but needed to be integrated and made broadly and rapidly available to researchers. Unprecedented amounts of data sourced from public health surveillance were put to varied uses. These included vast amounts of real-time monitoring of outbreaks, the analysis of current and forecast trends, and analysis of news reports and organizational briefings about utilization. Numerous heterogeneous information systems were used by institutional researchers and hospitals capturing virological, epidemiological, and clinical characteristics. This resulted in fragmentation and the creation of multiple interoperable data "silos."

[10]For example, the OBO Foundry (Jackson, Rebecca et al., 2021).

Rapid identification of a data integration problem quickly led to standardization efforts, starting with data about infections. In the OBO Foundry the Coronavirus Infection was formally defined using concepts from an aligned suite of modular interoperable ontologies. These include the Infectious Disease Ontology (IDO) and the Chemical Entities of Biological Interest (ChEBI), as well as the Human Phenotype Ontology for human host phenotypes. Updated standardization for COVID-19 was guided and simplified by the use of semantic resources and incorporation of knowledge organization systems (taxonomies and vocabularies as well as OBO ontologies) as background knowledge. This started with designing a common space that included a standard vocabulary defining the symptoms of a "Coronavirus Infection:"

> is characterized by fever, cough and shortness of breath and that has a material basis in SARS-CoV-2.

This definition can easily be found in trusted places, based on sound principles and practices like the OBO-Foundry. It can also be found using special ontology search engines such as the Ontology Look up Service (OLS) or the European Bioinformatics Institute (EBI-EMBL). The standard definition found in these sources includes a common identifier that is not only in ontologies and Wikipedia, but is axiomatized throughout the OBO Foundry. Using OLS we find the same (unambiguous) concepts cross referenced in different access tools. Along with other material it can be found in the following:

url:https://www.cdc.gov/coronavirus/2019-ncov/about/index.html
url:https://www.ncbi.nlm.nih.gov/pubmed/?term=32007145
url:https://www.ncbi.nlm.quadih.gov/Taxonomy/Browser/wwwtax.cgi?id=2697049

To flesh out the COVID-19 model some vocabularies of the core IDO model were enhanced by introducing the metadata/ontology vocabulary item *acellular*. This captures the idea of a structure to cover viruses along with *other acellular entities* that are studied as part of virology. These allowed distinguishing between *infectious agents* (i.e., organisms with an *infectious disposition*) and infectious structures (i.e., acellular structures that have an infectious disposition). Several new extensions in IDO virus ontology (VIDO) (Babcock et al., 2021) and the Coronavirus Infectious Disease Ontology (CIDO) (He et al., 20210) were developed and aligned with part of IDO so these ontology modules shared the same vocabulary (e.g., the

concept of *Symptom*). Together these were designed to align and provide broad coverage across various aspects of the infectious disease domain such as allowing simple extensions to new pathogen-specific ontologies, which helped identify drug candidates that could be repurposed for an effective and safe COVID-19 treatment. Over 90 chemical drugs and antibodies against human coronavirus diseases were identified early on by mapping anti-coronavirus drugs to ontology identifiers from ChEBI and drug data using semantic similarity analysis (Liu et al., 2020).

This work shows the role of extendable modular domain ontologies working together to support interoperability at both the data and ontological level. The common OBO metadata also support other semantic resources like the creation of KGs which put diverse data together. It also illustrates the incremental way that modular ontologies may be matured over time (Berg-Cross, 2022).

5. Conclusion and Challenges for Grounding Metadata

We have seen some challenges pursuing shallow, objective grounding of concepts for approaches like FAIR maturity indicators. In the case of data these rely on too simple and shallow a semantic view of operationally defined meanings. In conclusion we can understand some of the problems of meaning that arise because of the recursive design considerations for the FAIRness evaluation framework. This reflects the insistence that all components of the evaluation framework should themselves be FAIR and would apply across the full range of digital forms of semantic resources. Most notably they apply to controlled vocabularies and taxonomies used to play the role of metadata along with ontologies that also play an important role in making metadata FAIR. These all need to be FAIR. However, generating a semantic model is often the most time-consuming step of what goes into systematically making data and metadata FAIR (Jacobsen et al., 2020). Moreover, users have to find and access a relevant ontology first to support this type of interoperability. But domain ontologies typically don't fully cover domain user interest or provide meta-ontology links to connect relevant ontologies; and, as we have argued, there is often the issue of alternate ontologies as well as other forms of semantic resources that might provide additional, possible conflicting information. Although ontologists have developed several guiding principles for documenting ontologies, finding and developing the range of resources needed for proper scoping and

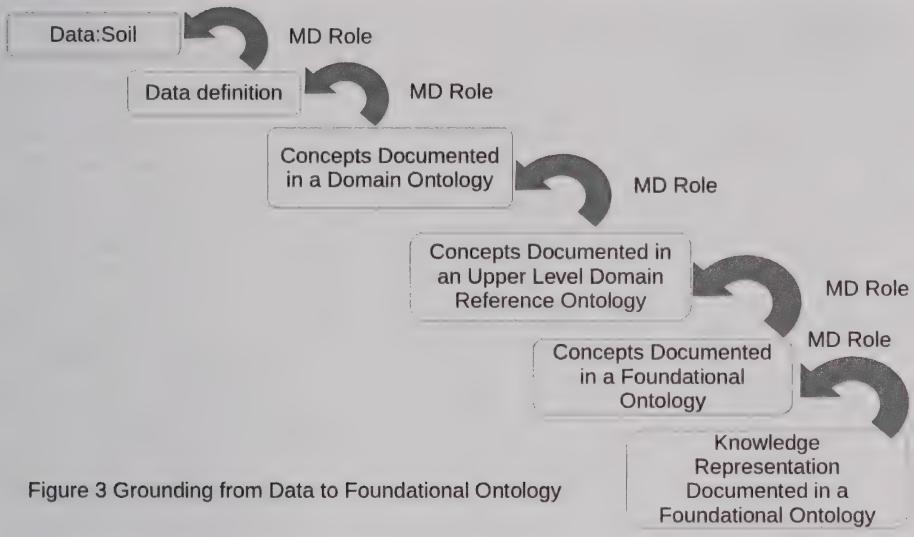

Figure 3 Grounding from Data to Foundational Ontology

coverage can be difficult for ordinary users. Grounding a whole suite of semantic resources using a meta ontology is still more difficult.

Metadata play a key role from finding to interoperation. An example is the diversity of conceptualizations of soil that was mentioned previously. What might be a simple example of rich metadata usable to start formally disambiguating many alternate definitions? One might think that the source for this richness is found in the related schemas of ontologies. However, these axiomatized schemas need to be grounded in community agreed upon conceptualizations rather than arbitrary semantic resources expressed in various ways. One can start with a domain ontology as shown in Figure 3, and one can point to an example of an axiomatized schema for soil in ENVO used as a previous example. The richness of an axiomatized definition relies in part on further definitions of terms and their axiomatizations supporting the soil definition. Thus "porous" is further defined in text as "a porosity quality inhering in a bearer by virtue of the bearer's being capable of admitting the passage of gas or liquid through pores or interstices." In this way rich metadata becomes more richly connected, replacing simple value pairs with a complex axiom pattern, which are, in turn, grounded in rationalized and useful definitions agreed upon by a community. There is a clear illustration of recursion of semantic grounding in such examples.

Having a common meaning is central to grounding, which implies that we need some better requirements for the grounding of meta ontologies. The concept of "porosity", for example, is not axiomatized in ENVO (2002). But some upper domain reference models do offer a range of basic concepts that might suffice for such grounding. These use basic concepts of containers and voids (Brodaric and Hahmann, 2014; Brodaric, Hahmann, and Gruninger, 2019). As shown in Figure 3 this takes us one step further in grounding, and this can be further grounded in something like the Unified Foundational Ontology (UFO) (Guizzardi et al., 2022). The UFO combines theories from philosophical reasoning about formal ontology with cognitive science and linguistic theory. Operationally it is composed of a handful of micro-theories that cover fundamental conceptual modeling notions such as kinds, primitive types and collectives. Still more grounding can be obtained by including concepts to describe the type of class a "kind" is and to detail meta-relationship (logical) types like "reflexivity" and "symmetry".

Some decisions on grounding may be found by studying conversations within a community and/or by a fiat decision that can be defended practically. In other cases physical observations may be used, and objective rules may be established.

Some ontology management activities may be needed as a result of search activities. In practice, when a simple search for terms of interest within an identified, relevant ontology is unsuccessful, new ontology terms are often defined and added to the existing ontologies. But this must be done cooperatively so that related ontologies and their users are aware of the changes. If the structure of an existing ontology seems unsuitable, new ontologies may have to be developed. An example of this is the existing mismatch between the SWEET and ENVO ontologies, which were independently developed and which have very different structures (Pouchard and Huhns, 2014; Karam at al, 2020). However, this is a time-consuming process that often needs to be undertaken with a team of domain experts in consultation with ontology experts.

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Toward an Ontology for Third Generation Systems Thinking

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Aisystant

Abstract

Systems thinking is a way of making sense about the world in terms of multilevel, nested, interacting systems, their environment, and the boundaries between the systems and the environment. In this paper we discuss the evolution of systems thinking and discuss what is needed for an ontology of the current generation of systems thinking.

1. Introduction

SYSTEMS THINKING is a way of making sense of the complexity of the world [1]. Rather than only looking at individual parts, systems thinking takes a more holistic approach in which the world is viewed in terms of multilevel, nested, interacting systems, their environment, and the boundaries between the systems and the environment. Idealistically, the goal is to develop best practices for systems that will change the world for the better. Developing such best practices requires that individuals from many specialized disciplines both understand the systems and communicate with one another in a meaningful and useful manner. The notion of an ontology was developed as a means for supporting such interdisciplinary communication and for helping to better understand subject areas as well as many other purposes. In this paper we survey the generations of systems thinking. We then discuss the requirements for an ontology for the current generation of systems thinking.

We begin in Section 2 with some background in basic ontology and epistemology that will be used for describing systems thinking concepts. Section 3 discusses the first generation approaches in which a system is described within its environment as it is operating. Section 4 then discusses the second generation approaches which are concerned with the creation of a system-of-interest by systems that construct and enable other systems. The current generation of systems thinking is then described, starting with continuous development techniques in Section 5. Scaleless system descriptions are covered in Section 6, Section 7 is concerned with systems that perform operations on both physical objects and abstract objects. Sec-

tion 8 speculates on how the evolution of systems can be explained using thermodynamic principles. The paper concludes by summarizing the most important requirements of an ontology for third generation systems thinking.

2. Systems Ontology and Epistemology

An ontology is a way to express what a subject area represents by defining a set of concepts and categories as well as how the concepts and categories are related to each other. An ontology should indicate the objects that would be good to distinguish in the world for reliable active/embodied inference within the subject area [2]. We formulate the task of creating an ontology in terms of attention management, and "explicit formal specification" which here indicates that these objects of attention are not spontaneously singled out but according to some explicit model as ontology specified by using another model as its formalism (such as one of the foundational ontologies).

We resolve the issue of creating an ontology according to Popperian epistemology [3]: objects in an ontology appear by guessing, the acceptability of these guesses for judgments about the world is questioned, but guesses that survive criticism are "taken seriously." Good guesses about how the world is made up of systems (what is the ontology of the system) and judgments that these guesses help change the world for the better can be taken from current literature. Suppose we do not know their critique and cannot immediately suggest falsification of those conjectures by reasoning and/or experiment. In that case, we consider them our best theories (i.e., the state-of-the-art) about the world, take them seriously and then teach people (replicate memes of those theories) to make those conjectures about the important objects shared.

Of course, we do not just tell people the systems ontology. However, we teach them to attend to abstract and physical objects in the world, described by shared explicit and as formal as possible specification, i.e., ontology. Problems emerging within an activity performed with this ontology as a theory of the world mean that ontology is falsified, but this is simply a reason to correct the ontology by correcting identified errors. Systems ontology thereby continuously evolves. It represents at each point in time the best we know about systems at that point. We [4] have implemented a curriculum in which several hundred people a week are now learning to

identify in the world objects described/typed by systems ontology. The curriculum implements teaching students fully conscious at the start and then interiorized "automatic" conceptual guidance of students' attention to objects described/typed by systems ontology. The student is trained to:

- to direct one's own and other agents' attention to objects from an explicit specification (ontology), that is, to direct attention conceptually rather than spontaneously (Ontology and Communication course),
- to hold conceptually guided attention on a wide variety of time scales, including collective attention in such agents as a team and whole enterprise via leadership, or influencing on community or society (Self-Collectedness course),
- to direct attention to systems (Practical Systems Thinking course),
- to direct attention to the activities/practices that are carried out by constructor/enabling systems (Methodology course),
- structure the activities and roles that are necessary to be held in attention in the course of systems engineering projects (Systems Engineering course),
- to draw the attention of oneself and the team to the objects described by the systems ontology specialization for systems-creators such as organizations/businesses (Systems Management course).

To teach students a state-of-the-art systems ontology, we have harmonized several particular conceptualizations of the concept of systems (i.e., we performed a merge of partial systems ontologies), which after merging, represent together an ontology of the third generation of systems thinking. As usual, each generation of systems thinking incorporates all the previous generation's achievements but adds something new.

3. The first generation approach

The first generation of systems thinking emerged in the 1940s, mainly as a result of the work of von Bertalanffy [5]. The notion of a system as a subject separated from its environment appeared in physics long ago. However, the systems approach as a consideration of the whole world as interacting systems appeared mainly after von Bertalanffy's works on general systems theory. "Approach" is the usual term for a situation in which ontology, successfully developed and tested in one domain, begins to

be used in many different domains. The key here was the realization that systems are interacting holons (Koestler coined the term [6] to describe a part of the whole that itself is made up of parts). Also, these systems somehow appear in the world and then disappear from the world during a life cycle (von Bertalanffy was a biologist, and he generalized, among other things borrowed from the systems approach in biology, that the life cycle is the birth-growth-breeding cycle). The interaction of parts of the system during work/operations results in emergent properties of the whole. The gears in the clock do not yet show the time, the clock shows the time, and the house with the clock inside no longer shows the time. The key here was that the first generation of systems thinking operated on at least two different ways of partitioning depending on the time of consideration:

- functional partitioning depends on the system's purpose in the suprasystem and the subsystems in the system. This viewpoint needed to think about the system during its operations in its environment.
- a constructive/modular partitioning is needed to think about the system at the creation/construction time.

The difficulty in mastering systems thinking was that people needed help grasping the concept of selecting/isolating dynamic objects in the world with their attention to the system at operations time. Often, they imagine an "explosion diagram" in their heads when mentioning decomposition into functional parts, simultaneously losing the multiple system levels of such a partitioning [7]. Mereology is the study of parts and the wholes that they form. One cannot discuss the emergent properties of the stopped broken-down system into single-level physical constructive parts because interaction happens in operations time, and viewpoint must be functional, not constructional. Nevertheless, partitioning into constructive parts is also essential, for such a system must be created in construction (design, implementation, test, deployment, transfer to operations) time. For example, scissors functionally consist of a cutting unit and a handle, while structurally, for construction, they consist of two halves of scissors and a screw that fastens them together. The scissors user is concerned with the functional viewpoint, while the factory engineer is concerned with the constructional viewpoint.

Bertalanffy included systems engineering in his proposed set of sys-

tems disciplines. The field of systems engineering subsequently developed rapidly. In systems engineering, the target systems were physical, which has the advantage that all descriptions have a guaranteed grounding. However, it proved to be impossible to go beyond mereology to more abstract notions such as the relations between whole objects, parts, parts of parts and boundaries between parts. The study of such relations is called mereotopology. Attempts to develop a mereotopology of mental/abstract/mathematical objects that comprise views mostly failed.

4. The second generation approach

The second generation of the systems approach relied mainly on the ideas of systems engineering: physical (including cyber-physical, including cyber-physical with people) systems-of-interest are created by people with tools, not reproduced themselves in a cycle, and usually non-living. The notion of the life cycle turned out to be neither life nor cycle, although the term for the concept remained in use. In the second generation of the systems approach, constructor/enabling systems appeared. That introduces, besides the part-whole relation, the construction/enabling relation and the viewpoints for the activity of constructor systems and interaction of constructors and systems-of-interest (the most famous introduction of this viewpoint was works of Checkland in the late 70s and early 80s [8]). Systems engineering was supplemented with systems engineering management from the viewpoint of construction/enabling systems, thus enabling a chain of constructors and enablers (i.e., constructors of constructors of systems-of-interest).

The systems engineering diagrams emphasized the "waterfall" model of the life cycle, in which the system was conceived, designed, implemented, tested, operated, and decommissioned, where the project usually ended. The living system does all this work for itself by itself (with some conceiving and design work done for them by evolution, but this was not usually considered). However, in engineering, it was all done by the constructor as a separate system. Different roles (stakeholders) in the project-as-the-constructor-chain have different interests/concerns for the system and the project. These concerns require different kinds of descriptions/views that should be made with respective viewpoints as methods of system description that suit to reconcile the very different concerns of the very different project roles.

The ISO 42010 [9] and ISO 15288 [10] standards solidified the conceptualization of the system for systems engineering. Wide usage of these standards ensured that the second-generation systems engineering ontology of the systems approach was shared. A formalization of systems ontology based on 4D extensionalism (the idea that if two objects occupy the same place in space-time, they are the same object – and it is a physical object) was proposed in ISO 15926-2 [11] in 2003. It drew on ideas from the Business Objects Reference Ontology [12]. Based on this 4D ontological commitment, several other similar ontologies were proposed mainly for military applications. This work was led by the IDEAS Group [13]. Special mention can be made of the work of Matthew West, who proposed the High Quality Data Models ontology based on the same ideas of 4D extensionalism [14], in which the concept of the system was made one of the central ontologies. All these approaches assumed not just conceptualization specification but also a formal expression of conceptualization. This formalization can be done with logical ontology description languages (such as the very rarely used EXPRESS language [15] but also appeared later more popular Web Ontology Language (OWL) [16]) to create data models in Product Lifecycle Management (PLM) systems databases [17]. The fundamental ontological premise was to use a 4D ontology, which gave a reasonable and compact description of the system's changes during its construction from parts [18].

The peak of this line of work on the second generation of the systems approach that evolved in systems engineering came in 2008-2013. After that moment, public interest in such logic-based formal systems ontology descriptions faded a bit. The development of ontologies as an explicit formal specification of shared conceptualizations was no longer seen as an advance in AI creation, and not even the rebranding of formal ontologies as knowledge graphs helped [19]. The semantic web was expected as an internet mainstream Web 3.0, but this idea was never realized. Semantic technologies remain niche.

5. Continuous development

The "waterfall model" [20] was the limited idea of a single unidirectional passage of the life cycle as a set of works carried out by constructors following life cycle practices. System-of-interest was considered as passively undergoing this one-time creation. Therefore, agile approaches were devel-

oped in engineering, overcoming the concept of a "waterfall" life cycle. In 2001 the Manifesto for Agile Software Development appeared [21]. In 2017, evolvability as a core architectural characteristic reflecting the "continuous everything" notion was entrenched in best engineering practice and entrenched in the literature [22]. The architecture was finally separated from development into a separate domain as the literature began to reflect the inevitable "productive conflicts" between architects and developers. Architecture worked on slicing the system into minimally interacting modules to maintain the stability of the whole in the evolutionary time scale (maintain characteristics such as -ilities well known in engineering appear as architectural characteristics). At the same time, developers were concerned with maximizing functionality, which could entail temporary deterioration of architectural characteristics as an accumulation of "technical debt" (work aimed at maintaining selected architectural decisions but not directly affecting functionality).

The idea of evolutionary cycles was introduced to engineering, but in a different way from biological evolution because the systems memome, as an analog of the biological genome, was not contained in the manufactured system but was separately stored in a digital form somewhere in the constructor systems. Digital form implies exact multiple replications without accumulation of errors of analog representation. The separation of the memome and the system defined by that memome significantly speeds up the techno-evolution compared to the biological one. For some techno-crab, it was not necessary to wait until the whole crab died to replace the unsuccessful claw variant only with the crab as a whole by mutations of genes forming the phenome of the claw. It was also possible to use smart mutations to techno-crab memome, getting quicker and more reliable results. It is possible to try only claw variants that showed success in simulations in the virtual world – and to change in real life only the claw, but not the whole crab, especially if the system has a proper architecture with good modularity. Techno-evolution gives results unattainable only by a one-time offer of a set of new features (one-time "waterfall" engineering) or only evolution with random mutations [23]. System modeling at operation time practice was adopted with a digital twin to assess the system's success in its operations. The concept of a digital twin reflects not only the memome but also the phenome of the system. So a systems ontology focused on two times (1. operation and 2. creation of a single increment/feature)

was not enough. It was also insufficient to model a whole group of systems (product lines [24], sometimes system families) as different system variants coexisting.

The way out was the idea of "continuous everything" [25] as infinitely ongoing system development with continuous delivering and commissioning of more and more variants of the target system with more and more changes for fit to environments. Slowing down development with the growth of system-of-interest complexity in continuous delivery is suppressed both by the evolving architecture and the changing structure of the teams that perform this development (using Conway's inverse maneuver [26]). In software engineering, this idea appeared within the DevOps/SRE/platform engineering approach [27]. In traditional systems engineering, this idea is discussed now in examples of aerospace systems. Testing of the next version engines nowadays starts before the tested engines of the first version in the rocket perform their first flight, and each new instance of rocket hardware has an improved design. "Continuous everything" means moving engineering to techno-evolution projects, that is, evolutionary changes in the meme – continuously improving the information model of the system design, not just the improving phenome by "field refinement" of an instance of the system. Continuous development as the practice of techno-evolution tries to endlessly keep system-of-interest, adapting it as long as possible to changes in the environment, in itself, and changes in a chain of constructor systems. In biology and life sciences, similar problems of approaching infinite in time development/techno-evolution are discussed as open-endedness [28].

Thus a requirement to reflect the ideas of evolution in systems ontology emerged. Suppose there was a developed ontology of evolution. In that case, it could be used to develop a third-generation systems approach that would account not only for construction/enabling systems as agents in their different project/activity roles but also for techno-evolution. It would work explicitly with three times:

1. Operations time of the instance of a system with intended by design phenome
2. Construction time of a system instance with an increment change in design, i.e., phenome from memome implementation

3. Continuous changing of memome time (techno-evolution, continuous everything)

6. Scaleless descriptions of physical systems

In the discussion of evolution in biology, the systems approach manifested itself in reality in major evolutionary transitions: increasing complexity in systems from large molecules to cells, from cells to multicellular organisms, and from organisms to populations. Approximately the same increase in the complexity of systems occurs in techno-evolution: chips are composed of transistors, cards of chips combine to form computers, stacks of computers aggregate to form data centers, and data centers transit to global computer networks. The analogy seems straightforward but requires a scaleless theory that will be common for systems of any scale and origin. Such a theory should be valid for the world of elementary particles in nuclear physics (taking into account quantum phenomena) but also for macro-objects, including living and non-living, as well as living conscious beings and collections of living conscious beings (for example, humankind as a whole). Scaleless also meant scaleless in the fourth dimension, time: considering the system construction/growth time, operations time, and evolution time.

A key step for developing scaleless descriptions is to formulate physical phenomena in informational terms and to explain how some objects remain stable in the physical world. How do some objects (such as a molecule or a person) maintain their shape in space-time? Fields, Glazebrook, Levin, and Friston proposed an ontological framework of panpsychism in a variant of minimal physicalism to describe physically persistent systems as the realization of the principle of free energy minimization [29]. Their theory covers the complexity spectrum from elementary particles to people and society. Free energy is defined as an informational characteristic of a system rather than the traditional energy of mechanical work or the work of electromagnetic forces. These systems increase in complexity from elementary particles through molecules, through inert matter bodies to living cells, and from unicellular to multicellular organisms and their populations. All of these types of systems reduce the Bayesian (or excess Bayesian to account for the quantum-like nature of computation in biology [30]) surprise of mismatch between expected measurements according to a generative model of the world and actual measurements in the world.

This scaleless ontology for physically persistent systems has been mereologically formalized using category theory as a foundation ontology [31, 52] and expressed in a form that allows describing quantum-like active/embodied inference [32]. This line of ontological engineering provides concepts for accurate reasoning about systems of very different evolutionary complexity, including applying stochastic methods to non-ergodic systems, that is, systems with memory. One of the strongest confirmations of such a theory was the creation of a learnable hybrot [33]. Hybrot, as a sufficiently complex system capable of learning (such as a natural neural network), must exhibit (due to the principle of free energy minimization) behavior that minimizes the unpredictability of the external environment. Precisely that was shown by experiment, hybrot learned to play Pong [34]. This line of research achieved the formalization and mathematization of ideas of the first generation of the system approach in physics-based ontology. Due to the scaleless nature of this ontology, other time scales also can be covered: the time scale of a system's life cycle and the time of evolution. The key to this was the notion of measurement, developed in quantum physics to solve the problem of the observer. Measurement is an interaction of systems, not just passive perception/observation. The reverse is also true: the interaction of systems in the construction process is described as the inverse of measurement. Any molecule's interaction as a system with its environment can be considered either a measurement or construction. A molecule is a proto-agent that somehow perceives/cognizes/measures the world around it, maintaining its stability while obeying the principle of minimizing free energy.

This line of reasoning (perception/measurement as inverse to changing/constructing, and both are an interaction of systems) was drawn in the constructor theory proposed by Deutsch and developed by various researchers of "quantum gravity" that needed scaleless theories [35]. A constructor is a physical device that can maintain its immutability for a long time while repeatably changing its environment by some pre-described sequences of operations. Examples can be a catalyst molecule, a robot with a universal computer, or a living being. Sufficiently advanced constructors can replicate themselves, among other things, to be the subject of evolution. Scaleless physical theories are based on notions of information-related changes as computations have proven to be very productive.

7. Constructivism

The next thing to be considered in the physics-based system ontology is the ontology of physics and mathematics itself as a foundation ontology. Such an ontology has been proposed in many works, but let us highlight the work of Deutsch [36]. He proposed to consider physics as a study of physical (situated in space and time) objects, mathematics as a study of mental/abstract/mathematical objects, and computer science as the natural/experimental science of proving that the behavior of physical objects can somehow reflect the behavior of ideal/abstract/mathematical objects. Computer science, according to Deutsch, is the science of universal computers as physical devices capable of performing computation – traditional electronic, quantum, and many other types, including biological and social computers such as the human brain and even collectives of humans altogether with their computers.

These ideas imply a shift of the discussion from static models and passive data to universal computers as physical devices that interpret such data and change the state of the environment depending on these computations. The input of raw data for computations and output of results in the symbolic form is just a particular case here. Perception of the environment and changing the environment and/or "self" as a computer/constructor device/system is just a more general case. Central to this approach will be the notion of a constructor. This physical device can interact with the environment, repeatedly performing some operations upon the objects in the environment while maintaining its stability (e.g., a catalyst molecule, a robot, or a human). So, we have some approach to a formal description of systems of the second generation of the systems approach: some systems of different degrees of agency (from inert matter, robots, intelligent agents, and all kinds of their hybrids) construct according to some design and method data, different types of systems-of-interest, which further operates in their environment.

One more attempt at integrating physics, topology, logic, and computer science with a shift of attention to enactive operations/morphisms with objects instead of considering static objects in their static relations was proposed by Baez and Stay in the Rosetta stone approach [37]. After moving from describing system interactions as processes in networks, Baez proposes to use the formalism of symmetric monoidal category theory to describe not just processes but open systems interacting with the environ-

ment [38]. Networks such as electrical circuits, hydraulic networks, and network interactions in system dynamics are usually associated with functional representations of the systems, that is, representations of the system in its environment in operations time, the first generation of the systems approach. Again we see a move to use category theory as a foundation ontology for systems ontology to represent it not as a set of static objects and relations but as morphisms as object changes. This move corresponds to a general move toward constructivism in mathematics, where we change eternal classes and their relations to construction operations [39]. This move makes it possible to reformulate mereology as the central ontological discipline of the systems approach from the study of the objects in "part-whole" relations [40] to the study of the operations of constructing a whole from parts.

Another move in this direction of constructivist mereology is Fine's ideas about the mereology that includes abstract objects [41], which suggest operations of constructing the whole from parts. Operations of constructing the whole from parts also apply to descriptions (constructing a set from its elements). Although Fine does not explicitly say so, defining construction operations (as well as category theory morphisms) performed as if by "nobody", but behind these constructor operations in the physical world, one can easily see a physical device that is the constructor from constructor theory. For the constructor of the whole for abstract parts, there will be a physical device implementing a "universal computer". It is also a constructor from constructor theory, including quantum computers and living mathematicians – they are computationally equivalent and physically embodied to get information about input and output data of computation. Fine's approach allows us to extend the notion of a system beyond physically interacting parts. Interaction of abstract objects appears inside computer devices as physical parts of computers interact to emulate abstract objects. The definition of a system as interacting parts with emergence persists, but interaction appears in the constructor/computer system rather than in the abstract system-of-interest. It is possible to discuss systemicity in complex communities in the physical world despite the absence of the interaction of the members of these communities with each other. The interaction of community members occurs by carrying out operations of reasoning about these communities in the constructor's computer (e.g., social engineer's brain) [42].

Core Constructional Ontology [43] is based on ideas of Fine and offers a constructivist perspective on the theory of parts, sets, and relations. Core Constructional Ontology serves as the second layer of foundational ontology for systems descriptions in a PLM system of engineering projects. For core constructional ontology first layer of foundational ontology is mathematics. 4-Dimensionalist Top Level Ontology expressing 4D mereotopology of space-time gives us the next ontology layer as an upper ontology for modeling physical systems in current systems engineering [44].

Using some mathematics as the foundational ontology is typical for computational ontology in the form of variants of first-order logic. However, more and more often, foundational ontology is based on morphisms and, respectively, category theory. Using mathematics as the foundational ontology and omitting all other (upper ontology, middle ontology) ontological levels are typical in physics. Physics itself, in terms of systems ontology, deals with functional objects (e.g., "physical body") whose roles are played by different objects of the physical world (mountains, stones, molecules, elementary particles). Then in conjectures and experiments, the peculiarities of behavior of these functional objects are found, and mathematical relations express them. Structural similarities of formulas describing some different objects raise the question about the general ontological nature of these objects. Thus ontology merges can be performed by analogical reasoning with ontologies represented by mathematical formulas. This technique is also used for ontologies expressed logically as lattices (knowledge graphs), an example of which is the VivoMind Analogy Engine [45]. The usage of such a technique by physicists is ubiquitous. E.g., in works on information theory, "free energy" is called so due to its appearance at the same place in similar formulas in informatics theory that it appears in formulas of thermodynamics [46]. The trend is to use mathematical/abstract objects and formulaic relations between them to formulate a third-generation systems ontology. Then we get the physical explanation of evolution with imminent major evolutionary transitions leading to multiple system levels in persistent objects.

8. Thermodynamics of system evolution

Vanchurin, Wolf, Koonin, and Katsnelson observed that analogy reasoning with classical thermodynamics and information theory, quantities in thermodynamics, machine learning, and evolutionary biology lead to

a surprising common framework/ontology for all of it [47]. In other words, evolution could be described as learning, and learning has thermodynamic nature, i.e., physical phenomenon. Based on these notes, they formulated the theory of evolution as multilevel learning [48]. In this theory, the driving force behind evolution is frustrations arising from conflicts between objects of different system levels. This notion of frustrations was introduced into the systems language by studies of spin glasses as an example of the behavior of non-ergodic (with memory) systems. It meant frustrations analogous to geometric frustrations as the impossibility of stable geometry of spins in glasses [49]. Evolution is thus a learning process, which is reduced to solving the optimization problem of finding a minimum of the free energy by changing the structure of numerous system layers. In the course of this, evolution finds quasi-minima but not an absolute minimum. From time to time, there is a jump in complexity growth (appearance of another system level, another type of whole system, e.g., multi-cell organism constructed from cells), which gives a sharp minimization of the free energy of the evolving system. However, this is still just another quasi-minimum, not an absolute minimum. In [50], the physical/thermodynamical nature of the growing complexity of systems was shown with the example of biological systems. The reasoning there is scaleless, i.e., applicable to the living (with different degrees of consciousness and sentience), cyber-physical, and even inert systems. It means that systems ontology should include the notion of conflicts between system levels, the notion of the frustrations caused by these conflicts, and the rule (law, conclusion) of the inevitable growth of system complexity (inevitable increase in the number of system levels in the course of evolution).

Many of the aforementioned researchers are in contact with each other. Therefore, there is hope for a shared third-generation system ontology. For example, there were discussions between Vanchurin and Friston, which is indicated at least in the acknowledgment to [47]. Most of the mentioned works are based on thermodynamics and the premise that all systems obey the free energy principle during their existence, creation/construction, and subsequent continuous evolution. This systems ontology is currently expressed in the formulas familiar to physicists, traditional for thermodynamic calculations. The translation of the traditional formulas for expressing this ontology into the constructivist form of category theory is a separate topic. However, such a formulation of the problem is more or less

usual for mathematicians. We can discuss the research program on unifying mathematical languages used in different studies of the same domain of thermodynamic-based systems ontology. The same can be said about reformulating the differential form into a quantum-like form to increase the speed and accuracy of the physical modeling of biological evolution and techno-evolution [51].

9. Conclusion

An ontology for state-of-the-art third generation systems thinking should:

- provide types of objects for layered directing of attention to ensure the evolution of systems-of-interest (continuous everything) by constructor systems
- consider at least three times of system existence: operations, construction and evolution of phenome, evolution and development of genome and memome.
- be based on physics, mathematics, and computer science
- treat systems as stable entities within a minimalist physicalism (including systems active to themselves and their environment, systems seeking minimum free energy by active/embodied inference, regardless of their level of "intelligence")
- give scaleless descriptions of systems (phenomena of quantum physics are thereby taken into account), which explains the emergence of system levels (growth of complexity) due to multilevel optimization to achieve the minimum of free energy
- no longer express mereology through eternal classes and relations between them, but rather through morphisms and operations reflecting operations with physical systems in the course of their interaction as well as operations with abstract objects performed by constructor systems with a (universal in the sense of Turing machine equivalence) computers in them.

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Finding Transition Points
Zero-Crossings, Maxima, Minima and Inflections

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Abstract

A function has a transition point when some property changes at the transition point. Such points represent important features of a function. We examine three kinds of transition points: sign, monotonicity and convexity. A sign transition point, usually called a zero-crossing, is a place where the function changes from negative to positive or vice versa. At a monotonicity transition point the function changes from increasing to decreasing or vice versa. At a convexity transition point the function changes from being convex to concave or vice versa. When the function is continuous these three kinds of transition points are roots, maxima/minima, and inflection points, respectively. In this note we specify algorithms for finding the three kinds of transition points. We formally prove that the algorithms always converge, and we compare these algorithms with other algorithms. In the proof of the algorithm for inflections, we give a geometric interpretation of the mediant and its connection to convexity.

Introduction

A TRANSITION POINT is a place where a function has an abrupt change of some property. Formally, a function $f(x)$ has a transition point for properties P and Q at $x = x_0$ if there are real numbers $a < x_0$ and $b > x_0$ such that f has property P on the open interval (a, x_0) and has property Q on the open interval (x_0, b). Note that the function $f(x)$ is not assumed to be continuous, and the intervals where f has the properties P and Q do not include x_0[1].

We will consider three kinds of transition point as follows:

Sign transition point. The sign of the function changes from negative to positive or vice versa. Such a point is called a zero-crossing. When the function is continuous, the point is a root (zero) of the function.

Monotonicity transition point. The function changes from increasing

[1]Technically, the transition point is the point $(x_0, f(x_0))$ in the plane. For simplicity we will omit the reference to $f(x_0)$ and refer to x_0 as being the transition point.

to decreasing or vice versa. If the function is continuous, such a transition point is a local extreme point (i.e., a maximum or minimum).

Convexity transition point, The function changes from convex to concave or vice versa. If the function is continuous, the transition point is an inflection point.

Transition points are often confused with other kinds of points. For example, zero-crossings are commonly confused with roots. However, these two notions are different in general. Consider the following function:

$$g(x) = \begin{cases} 1/x & \text{if } x \neq 0, \\ 1, & \text{if } x = 0. \end{cases}$$

The function $g(x)$ is shown on the left in Figure 1. This function has no roots but has a zero-crossing at $x = 0$. Next consider the following function:

$$h(x) = \begin{cases} 1/x^2 & \text{if } x \neq 0, \\ 0, & \text{if } x = 0. \end{cases}$$

The function $h(x)$ is shown on the right in Figure 1. This function has a root at $x = 0$ but has no zero-crossings.

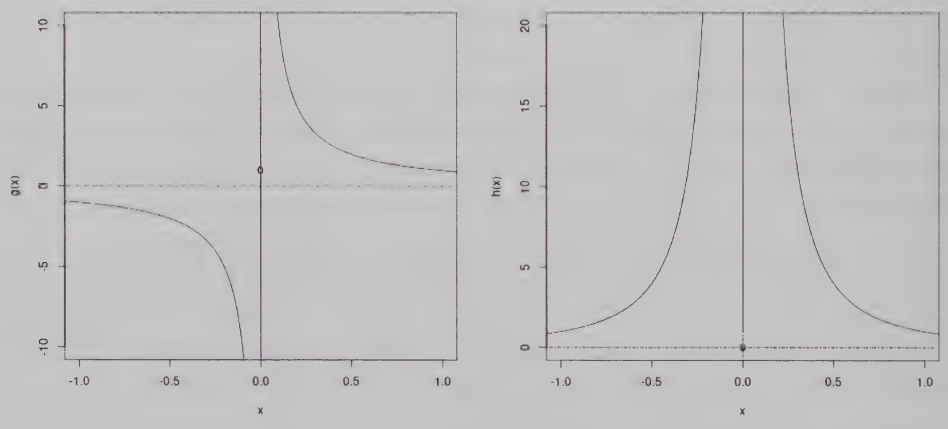

Figure 1: Left: A function that has a zero-crossing but no roots
Right: A function that has a root but no zero-crossings

The distinction between a root and a zero-crossing is significant since an algorithm for finding a zero-crossing would not be as effective in general for finding roots and vice versa. For example, the bisection method is often described as a method for finding a root of a continuous function when it is actually a method for finding a zero-crossing of a function that need not be continuous.

As another example, consider the following function:

$$k(x) = \begin{cases} x^2(1+\sin^2(1/x)) & \text{if } x \neq 0, \\ 0, & \text{if } x = 0. \end{cases}$$

The function $k(x)$ is shown on the left in Figure 2. This function has a minimum at $x = 0$, which is not a monotonicity transition point. On the other hand, consider the following function:

$$l(x) = \begin{cases} 1/x^2 & \text{if } x \neq 0, \\ 10, & \text{if } x = 0. \end{cases}$$

The function $l(x)$ is shown on the right in Figure 2. This function has a monotonicity transition point but has no minima or maxima.

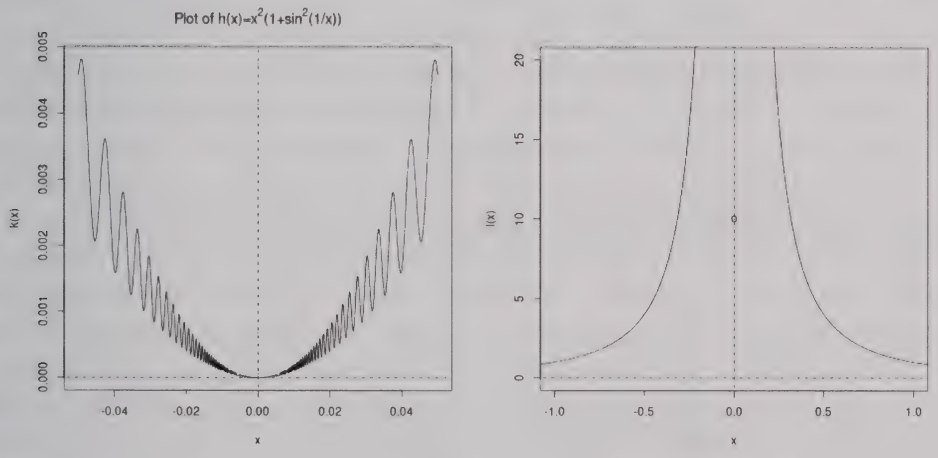

Figure 2: Left: A minimum point that is not a monotonicity transition point Right: A monotonicity transition point that is not a minimum or maximum

In any algorithm for finding a special point, the function and possibly derived functions will need to be evaluated. As computations will generally have limited precision, computed numbers can be indistinguishable from one another even though the theoretical numbers are different. In this paper we will write η for the accuracy of the computed function and any derived expressions. For two numbers y and z, we write $y \approx z$ to mean $|y - z| \leq \eta$, i.e., y and z are indistinguishable up to the specified precision.

We begin by describing the well-known bisection method for finding a zero-crossing. We then define bisection-style algorithms for finding monotonicity and convexity transition points. Each of the bisection-style algorithms are compared with other methods for finding special points of functions. In the Appendix we prove that the newly introduced algorithms are correct and therefore converge. One interesting feature of the proof of Theorem 2 is its use of the mediant for numbers other than integers. We also give a geometric interpretation of the mediant that visually shows its connection with convexity.

Zero-Crossings

There are number of methods for finding a zero-crossing. All of the methods start with an interval such that the function has opposite signs on the endpoints, and the methods iteratively reduce the size of the interval, which confines the zero-crossing to smaller and smaller intervals. The method terminates when the interval is smaller than a specified length or the function value is equal to zero within the precision of the computation of the function. This forces the zero-crossing to be within the final interval, up to the precision of the computations. Algorithms with the property that the desired point is always within an interval at each iteration are called *bracketing methods*. The simplest bracketing method is the bisection method, which simply splits the interval exactly in two at each iteration. Another bracketing method is the *false position* method, also called the *regula falsi* method. This method uses the intersection of the secant rather than the midpoint. The Interpolate Truncate and Project (ITP) method is an improvement of the false position method that adjusts the secant intersection in a number of ways that are determined by three parameters (Oliveira and Takahashi, 2020).

The performance of an algorithm for finding a zero-crossing is measured by the number of evaluations of the function. The bisection method

is optimal in the sense that its worst case performance is at least as good as any other algorithm for finding a zero-crossing (Sikorski, 1982). The bisection algorithm has the additional advantage that it is simple and requires very little additional computation beyond a function evaluation in each iteration.

While the bisection method has optimal worst case performance, the other bracketing methods can have much better performance on some classes of functions. Moreover, the ITP method is claimed to have the same optimal worst-case performance as the bisection method (Oliveira and Takahashi, 2020). However, it is worth noting that part of the reason why the ITP method achieves the optimal worst-case performance of the bisection method is that it defaults to the bisection method when it is unable to improve on the bisection method. Indeed, every algorithm for finding a zero-crossing can also achieve the same optimal worst-case performance as the bisection method by defaulting to the bisection method.

Every bracketing method requires one to specify the function f and the interval (a,b) where one is looking for a zero-crossing. The interval must be within the domain of the function, and the function must have opposite signs on the two endpoints of the interval. One must also specify the desired accuracy $\epsilon > 0$ of the zero-crossing point and the computational precision $\eta > 0$.

The are two cases for opposite signs. We refer to each one as the "pattern" of the zero-crossing that is to be found. The following is the method written in pseudo code:

Iteration:

1. Interpolation: Compute a point $c \in (a,b)$ according to the particular algorithm. For the bisection algorithm, $c = \frac{a+b}{2}$. For the false position algorithm, $c = \frac{af(b)-bf(a)}{f(b)-f(a)}$,
2. Search for Pattern: At least one of the pairs (a,c), (c,b) will satisfy the required pattern.
3. Replace the Pair: Select the pair that satisfies the required pattern and replace (a,b) with the selected pair.

Termination Conditions: There are two conditions for terminating the algorithm.

1. If $b-a \leq 2\epsilon$, then the midpoint $\frac{a+b}{2}$ will be within ϵ of the zero-crossing. This can be checked at the beginning of the iteration.
2. if $f(c) \approx 0$, then c is a zero-crossing up to the computational precision. This can be checked after c has been computed. The accuracy is $b-a$. Continuing the algorithm would not be useful since the function is too close to being a constant equal to 0 for the computations to distinguish the values from being 0.

Each step of the bisection algorithm requires a function evaluation and a small number of arithmetic operations. The length of the interval is reduced by a factor of 2 at each step, so the algorithm will always terminate in no more than $\left\lceil \log_2 \frac{(b-a)}{2\epsilon} \right\rceil$ iterations. Furthermore, if a function has a unique zero-crossing in the interior of the initial interval, then the bisection method will converge to it because every interval during the iteration will contain the zero-crossing in its interior. As discussed above, the other bracketing algorithms for finding zero-crossings can have better performance, but will have the same worst-case performance as the bisection algorithm if they default to the bisection algorithm.

There are other methods that can be used for finding zero-crossings. The secant method uses the same formula as the false position method, but does not check the sign of the function on the newly computed point and uses the newly computed point together with the most recently computed point for the next iteration. The secant method is not a bracketing method, and it can fail to converge to the zero-crossing.

Newton's method is a well-known algorithm for finding a root of a continuously differentiable function (Newton's Method, n.d.). However, it has a number of disadvantages compared with the bracketing methods. One must compute and implement the derivative of the function, so it is necessary to know the analytic formula for the function. Furthermore, Newton's method can converge slowly or even diverge, although one can mitigate this problem by monitoring the performance of Newton's method and defaulting to the bisection method when convergence is too slow. On the other hand, Newton's method can achieve high rates of convergence. For example, it can achieve quadratic convergence (i.e., the number of places in the approximation increases quadratically or better) when the function is twice continuously differentiable.

Monotonicity Transition Points

An extreme point (extremum) is one at which a function has a maximum or minimum. A frequently used method for finding an extremum is to differentiate the function and then find a root of the derivative. This is not quite accurate. A root of the derivative need not be an extremum. For example, the function $f(x) = x^3$ has derivative $f'(x) = 3x^2$ which is 0 at $x = 0$ but $f(x)$ does not have an extremum at $x = 0$. All one can say in general is that if $f(x)$ is differentiable and it has an extremum at x, then the derivative is 0 at x. The converse is not true. On the other hand, a function can have an extremum without being differentiable or even continuous at the extremum, as in the case of the function $l(x)$ shown in Figure 2.

We now define a method for finding a monotonicity transition point of a function, which we call the Bisection Monotonicity Method. The method has the advantage that it does not require one to differentiate the function. As with the ordinary bisection method above, there will be two patterns depending on whether one is seeking a minimum or a maximum. The algorithm proceeds as follows:

Input: Function f; three numbers a, b and c in the domain of f such that $a < b < c$ and such that either $f(a) \leq f(b) \geq f(c)$ (for finding a maximum) or $f(a) \geq f(b) \leq f(c)$ (for finding a minimum); a desired accuracy $\epsilon > 0$; and a computational precision $\eta > 0$.

Iteration:

1. Bisection: Compute the midpoints $d = \frac{a+b}{2}$ and $e = \frac{b+c}{2}$.
2. Search for Pattern: At least one of the triples (a,d,b), (d,b,e) and (b,e,c) will satisfy the required pattern. The proof that this search always succeeds is given in Theorem 1 of the Appendix.
3. Replace the Triple: Select any one of the triples that satisfy the required pattern and replace (a,b,c) with the selected triple.

Termination Conditions: There are two conditions for terminating the algorithm.

1. If $c - a \leq 2\epsilon$, then the midpoint $\frac{a+c}{2}$ will be within ϵ of the extremum.
2. if $f(a) \approx f(b) \approx f(c)$, then the function is constant in the interval (a,c) up to the specified precision, so no further processing can distinguish any of the points in the interval (a,c).

For both of the termination conditions, the midpoint $\frac{a+c}{2}$ will be within $\frac{c-a}{2}$ of the extremum. Both termination conditions can be checked at the beginning of the iteration.

In the Iteration step one could first try one of the midpoints, say d, and if $f(d)$ is greater than or equal to $f(a)$ and $f(b)$, then the pattern has been found without computing the other midpoint and its value. Accordingly, each step of the Bisection Monotonicity Method requires one or two function evaluations and a small number of arithmetic operations. Note that the initial triple (a,b,c) need not be equally spaced. However, if the initial triple is equally spaced, then all subsequent triples during the iteration will also be equally spaced. In this case, the length of the interval is reduced by a factor of 2 at each step, so the algorithm will terminate in $\left\lceil \log_2 \frac{(c-a)}{2\epsilon} \right\rceil$ iterations.

Furthermore, if f is a function on an interval $[a,b]$, and if $m \in (a,b)$ has the property that f is strictly increasing on $[a,m]$ and strictly decreasing on $[m,b]$ (or vice versa), then the Bisection Monotonicity Method converges to m. To see why this is so, first note that when a function is strictly increasing or decreasing, no triple will satisfy the pattern. So no triple during the iteration can be entirely within either $[a,m]$ or $[m,b]$. Therefore, every interval in the iteration contains m in its interior, and it follows that the sequence of intervals converges to m.

Convexity Transition Points

An inflection is a point at which a function changes from being concave to convex or vice versa. A frequently used method for finding an infection is to differentiate the function twice and then find a root of the second derivative. This is not quite accurate. A root of the second derivative need not be an inflection. For example, the function $f(x) = x^4$ has second derivative $f''(x) = 12x^2$ which is zero at $x = 0$, but $f(x)$ does not have an inflection at $x = 0$. All one can say in general is that if $f(x)$ is twice differentiable and it has an inflection at x, then the second derivative is 0 at x. The converse is not true.

We now define a method for finding a convexity transition point of a function, which we call the Bisection Convexity Method. The method has the advantage that it does not require one to differentiate the function. As with the ordinary bisection method above, there will be two patterns.

The algorithm proceeds as follows:

Input: Function f; four numbers $a < b < c < d$ in the domain of f such that either $\frac{f(b)-f(a)}{b-a} \leq \frac{f(c)-f(b)}{c-b} \geq \frac{f(d)-f(c)}{d-c}$ or $\frac{f(b)-f(a)}{b-a} \geq \frac{f(c)-f(b)}{c-b} \leq \frac{f(d)-f(c)}{d-c}$; a required accuracy $\epsilon > 0$; and a computational precision $\eta > 0$.

Iteration:

1. Bisection: Compute the midpoints $p = \frac{a+b}{2}$,$q = \frac{b+c}{2}$, and $r = \frac{c+d}{2}$.
2. Search for Pattern: At least one of the quadruples (a,p,b,q), (p,b,q,c), (b,q,c,r) and (q,c,r,d) will satisfy the required pattern. The proof that this search always succeeds is given in Theorem 2 of the Appendix.
3. Replace the quadruple: Select any one of the quadruples that satisfy the required pattern and replace (a,b,c,d) with the selected quadruple.

Termination Conditions: There are two conditions for terminating the algorithm.

1. If $d - a \leq 2\epsilon$, then the midpoint $\frac{a+d}{2}$ will be within ϵ of the convexity transition point.
2. If $\frac{f(b)-f(a)}{b-a} \approx \frac{f(c)-f(b)}{c-b} \approx \frac{f(d)-f(c)}{d-c}$, then the function is linear in the interval (a,d) up to the specified precision, so further processing will no distinguish any convexity properties in (a,d).

For both of the termination conditions, the midpoint $\frac{a+d}{2}$ will be within $\frac{d-a}{2}$ of the extremum. Both termination conditions can be checked at the beginning of the iteration.

In the Iteration step one could first try two of the midpoints, say p and q, and if one of the quadruples (a,p,b,q) and (p,b,q,c) satisfies the pattern, then it is not necessary to compute the last midpoint and its value. Accordingly, each step of the Bisection Convexity Method requires two or three function evaluations and a small number of arithmetic operations. If the initial quadruple (a,b,c,d) is equally spaced, then all quadruples in the algorithm will also be equally spaced. As a result, the denominators in a pattern will all be the same, and it will not be necessary to perform the divisions. In this case, the length of the overall interval is reduced

by a factor of 2 at each step, so the algorithm will always terminate in $\left\lceil \log_2 \frac{(d-a)}{2\epsilon} \right\rceil$ iterations.

Furthermore, if f is a function on an interval $[a,b]$, and if $q \in (a,b)$ has the property that f is strictly convex on $[a,q]$ and strictly concave on $[q,b]$ (or reversing convex and concave), then the Bisection Convexity Method converges to q. To see why this is so, first note that when a function is strictly convex (respectively, concave), the slopes between successive points are strictly increasing (respectively, strictly decreasing), and hence do not satisfy the required pattern. So no quadruple during the iteration can be entirely within either $[a,q]$ or $[q,b]$. Therefore, every interval in the iteration contains q in its interior, and the sequence of intervals converges to q.

Conclusion

We have introduced the transition point, a new kind of special point for real-valued functions of a single variable that can be useful for analyzing properties of such functions. We have also introduced bracketing algorithms for finding extreme points and inflections using bisections. The new algorithms have a number of advantages compared with other techniques, such as being guaranteed to converge and not requiring any additional effort such as differentiating the function one or more times. The only significant disadvantage is that the algorithms do not have as good a performance as other techniques. Furthermore, when using the other techniques, it can be useful to default to the newly introduced bracketing algorithms so that one has both higher performance for many cases and guaranteed convergence in all cases.

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Appendix

In this Appendix, we provide the proofs that the iterations of the algorithms introduced in this paper always succeed, and therefore the algorithms always converge. We first prove that the Search for Pattern step of the Bisection Monotonicity Algorithm always succeeds for the maximum pattern.

Theorem 1 *Let f be a function on the interval $[a_1, a_5]$, $a_3 \in (a_1, a_5)$, $a_2 \in (a_1, a_3)$ and $a_4 \in (a_3, a_5)$. If $f(a_1) \leq f(a_3) \geq f(a_5)$, then there exists $i \in \{1,2,3\}$ such that the inequality pattern $f(a_i) \leq f(a_{i+1}) \geq f(a_{i+2})$ holds.*

Proof. There are four cases depending on how $f(a_3)$ compares with $f(a_2)$ and $f(a_4)$.

1. $f(a_3) \leq f(a_2)$ and $f(a_3) \leq f(a_4)$. Since $f(a_1) \leq f(a_3)$, it follows that $f(a_1) \leq f(a_2)$. Therefore, $f(a_1) \leq f(a_2) \geq f(a_3)$ and the pattern with $i = 1$ holds.
2. $f(a_3) \leq f(a_2)$ and $f(a_3) > f(a_4)$. This implies $f(a_1) \leq f(a_2) \geq f(a_3)$ as in the first case above.
3. $f(a_3) > f(a_2)$ and $f(a_3) \leq f(a_4)$. Since $f(a_3) \geq f(a_5)$, it follows that $f(a_4) \geq f(a_5)$. Therefore $f(a_3) \leq f(a_4) \geq f(a_5)$ and the pattern with $i = 3$ holds.
4. $f(a_3) > f(a_2)$ and $f(a_3) > f(a_4)$. These two imply the pattern with $i = 2$.

Note that in the first case above, both cases $i = 1$ and $i = 3$ hold. In every case the pattern holds for at least one i and the theorem follows.

Reversing all of the inequalities in Theorem 1 above gives the result for the minimum pattern.

We now prove that the Search for Pattern step of the Bisection Convexity Algorithm always succeeds.

Theorem 2 *Let f be a function on the interval $[a_1, a_7]$. Partition $[a_1, a_7]$ into 6 subintervals with the sequence $\{a_2, a_3, a_4, a_5, a_6\}$. If $\frac{f(a_3)-f(a_1)}{a_3-a_1} \leq \frac{f(a_5)-f(a_3)}{a_5-a_3} \geq \frac{f(a_7)-f(a_5)}{a_7-a_5}$, then there exists $i \in \{1,2,3,4\}$ such that the inequality pattern $\frac{f(a_{i+1})-f(a_i)}{a_{i+1}-a_i} \leq \frac{f(a_{i+2})-f(a_{i+1})}{a_{i+2}-a_{i+1}} \geq \frac{f(a_{i+3})-f(a_{i+2})}{a_{i+3}-a_{i+2}}$ holds.*

The proof of the theorem will use the following operation:

The *mediant* of ratios a/c and b/d, where $cd > 0$ is the ratio $\frac{a+b}{c+d}$ (Mediant, n.d.). Although the mediant is only defined for ratios of integers, it is obviously meaningful for ratios of real numbers in general. The property of the mediant that we will use is the following proposition. This proposition is easily proved by multiplying by the denominators and by canceling the common term. There is a proof in Mediant (n.d.),

Proposition 1 *If a, b, c and d are real numbers such that $cd > 0$ and $\frac{a}{c} < \frac{b}{d}$ (respectively, $\frac{a}{c} \leq \frac{b}{d}$), then $\frac{a}{c} < \frac{a+b}{c+d} < \frac{b}{d}$ (respectively, $\frac{a}{c} \leq \frac{a+b}{c+d} \leq \frac{b}{d}$).*

Figure 3: A geometric interpretation of the mediant

The mediant has a geometric interpretation. Suppose that one has three points A, B and C that proceed from left to right in the plane, i.e., the x-coordinates of A, B and C are strictly increasing. Figure 3 shows an example. Then the slope of AC is the mediant of the slopes of AB and BC.[2] Geometrically, it is easy to see that the slope of AC will always be between the slope of AB and the slope of BC, which is the conclusion of Proposition 1. Moreover, ABC will be concave or convex depending on the order of the slopes of AB and BC.

[2]To be more precise, the ratio defining the slope of AC is the mediant of the ratios that define the slopes of AB and BC.

Proof of Theorem 2. For simplicity in the proof, we will write y_j for $f(a_j)$. There are 32 cases depending on how $\frac{y_{j+1}-y_j}{a_{j+1}-a_j}$ compares with $\frac{y_{j+2}-y_{j+1}}{a_{j+2}-a_{j+1}}$, for $j \in \{1,2,3,4,5\}$. For technical reasons, the comparisons for $j = 1,2$ are $>$ and $\leq$; whereas the comparisons for $j > 2$ are $\geq$ and $<$. To deal with the large number of cases, we group them into sets denoted by five inequality symbols or asterisks. For example, the set $\{>>\geq **\}$ denotes the set of cases in which

$$\frac{y_2-y_1}{a_2-a_1} > \frac{y_3-y_2}{a_3-a_2}, \frac{y_3-y_2}{a_3-a_2} > \frac{y_4-y_3}{a_4-a_3}, \frac{y_4-y_3}{a_4-a_3} \geq \frac{y_5-y_4}{a_5-a_4},$$

and the remaining two inequalities can be in either direction, so the set $\{>>\geq **\}$ has 4 cases in all.

Set 1. $\{>>\geq **\}$ Applying Proposition 1 to each of the first three inequalities gives the following inequalities:

$$\frac{y_2-y_1}{a_2-a_1} > \frac{y_3-y_1}{a_3-a_1} > \frac{y_3-y_2}{a_3-a_2} > \frac{y_4-y_2}{a_4-a_2} > \frac{y_4-y_3}{a_4-a_3} \geq \frac{y_5-y_3}{a_5-a_3} \geq \frac{y_5-y_4}{a_5-a_4}$$

In particular, we have that $\frac{y_3-y_1}{a_3-a_1} > \frac{y_5-y_3}{a_5-a_3}$. However, by hypothesis we have that $\frac{y_3-y_1}{a_3-a_1} \leq \frac{y_5-y_3}{a_5-a_3}$. It follows that none of the 4 cases in Set 1 ever occur.

Set 2. $\{** <<<\}$ Proceed as in Set 1 by applying Proposition 1 three times. As with Set 1, it follows that none of the 4 cases in Set 2 ever occur.

Set 3. $\{\leq> ***\}$ The first two inequalities imply the pattern with $j = 1$. There are 8 cases in this set, one of which is in Set 2.

Set 4. $\{* \leq\geq **\}$ The second and third inequalities imply the pattern with $j = 2$. There are 8 cases in this set, none of which are in earlier sets.

Set 5. $\{** <\geq *\}$ The third and fourth inequalities imply the pattern with $j = 3$. There are 8 cases in this set, two of which are also in Set 3.

Set 6. $\{*** <\geq\}$ The last two inequalities imply the pattern with $j = 4$. There are 8 cases in this set, five of which are in previous sets.

All 32 cases have been accounted for, and for every case that can occur, one or more of the inequality patterns hold. The theorem then follows.

Reversing all of the inequalities in Theorem 2 above gives the result for the other inflection pattern.

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Member News

We are pleased to announce that Life Fellow **Dr. Azad M. Madni** has been selected by the National Academy of Engineering to receive the 2023 Bernard M. Gordon Prize for Innovation in Engineering and Technology Education. He is being recognized for creating and disseminating a transdisciplinary systems engineering education paradigm based on entrepreneurial leadership, innovation, convergence, social awareness, and diverse thinking and backgrounds. https://bit.ly/3CN26vZ

Our Life Fellow and both Past and Future President **Dr. Ram D. Sriram** has received two awards:

• He is the recipient of the 2023 Honorary Member Award from the Institute of Industrial Engineers and Systems.

• He has been elected to the College of Fellows of The American Institute for Medical and Biological Engineering for outstanding contributions to federal health information technology research and programs.

Congratulations to Azad and Ram for their achievements!

We wish to welcome Fellow **Jorome T. Gibbon**, LSM IEEE, who is the new representative of the IEEE Northern Virginia Section.

Albert H. Teich
1942-2022

WAS Fellow Albert H. Teich died April 26, 2022, after a fall and ten days in intensive care in N. Bethesda, MD. He received his B.S. in Physics (1964) and Ph.D. in Political Science (1969) from MIT.

Professionally, Al was involved with science policy issues such as visa and immigration policy, research and development in the federal budget, climate change, and human rights. He was most currently a Research Professor of Science, Technology & International Affairs at the Institute for International Science and Technology Policy in the Elliott School of George Washington University in Washington, DC. Prior to joining the GW faculty, he was director of Science & Policy Programs for the American Association for the Advancement of Science (AAAS), where he was responsible for the Association's activities in science and technology policy for 32 years, managed a staff of about 40 people, and served as a key spokesman on science policy issues. He published Technology and the Future (originally Technology and Man's Future) in 1971, revising the compilation of essays through 12 editions, ending in 2012, and it remains in use as a coursebook of readings in science and technology issues.

While at AAAS he contributed to numerous articles and books, made innumerable presentations, testified multiple times before Congressional committees, and participated on advisory committees in the U.S. and around the world. He became a Fellow of AAAS in 1986, received an Award for Scientific Achievement in Science Policy from the Washington Academy of Sciences in 2004.

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Instrument Society of America	Hank Hegner
Marine Technology Society	Jake Sobin
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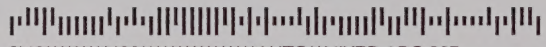

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